

# On the solutions of the Schrödinger equation with some molecular potentials: wave function ansatz

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February 1, 2008

## Abstract

Making an ansatz to the wave function, the exact solutions of the  $D$ -dimensional radial Schrödinger equation with some molecular potentials like pseudoharmonic and modified Kratzer potentials are obtained. The restriction on the parameters of the given potential,  $\delta$  and  $\eta$  are also given, where  $\eta$  depends on a linear combination of the angular momentum quantum number  $\ell$  and the spatial dimensions  $D$  and  $\delta$  is a parameter in the ansatz to the wave function. On inserting  $D = 3$ , we find that the bound state eigensolutions recover their standard analytical forms in literature.

Keywords: Bound states, pseudoharmonic potential, Kratzer's potential, Mie-type potential, anharmonic oscillator potential, Schrödinger equation, diatomic molecules

PACS number: 03.65.-w; 03.65.Fd; 03.65.Ge.

## 1 Introduction

The solution of the fundamental dynamical equations is an interesting phenomenon in many fields of physics and chemistry. To obtain the exact  $\ell$ -state solutions of

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the Schrödinger equation (SE) are possible only for a few potentials and hence approximation methods are used to obtain their solutions. According to the Schrödinger formulation of quantum mechanics, a total wave function provides implicitly all relevant information about the behaviour of a physical system. Hence if it is exactly solvable for a given potential, the wave function can describe such a system completely. Until now, many efforts have been made to solve the stationary SE with anharmonic potentials in three dimensions and two dimensions [1-5] with many applications to molecular and chemical physics. The study of the SE with these potentials provides us with insight into the physical problem under consideration. However, the study of SE with some of these potentials in the arbitrary dimensions  $D$  is presented in (cf. Ref.[6] and the references therein). Furthermore, the study of the bound state processes is also fundamental to understanding of molecular spectrum of a diatomic molecule in quantum mechanics [7]. The purpose of this paper is to carry out the analytical solutions of the  $D$ -dimensional radial SE with some diatomic molecular potentials by making a suitable ansatz to the wave function. These molecular potentials can be taken as pseudoharmonic potential [8,9]  $V(r) = D_e \left( \frac{r}{r_e} - \frac{r_e}{r} \right)^2$ , and a modified Morse or Kratzer-Fues potential [10-15] which is of a Mie-type form (cf. Ref. [14] and the references therein)  $V(r) = D_e \left( \frac{r-r_e}{r} \right)^2$  where  $D_e$  is the dissociation energy between two atoms in a solid and  $r_e$  is the equilibrium intermolecular separation. Morse potential [10] is commonly used for anharmonic oscillator. However, its wavefunction is not vanishing at the origin. On the other hand, the Mie-type and also the pseudoharmonic potentials [8,9] do vanish. The Mie-type potential [14] has the general features of the true interaction energy [16], interatomic and dynamical properties in solid-state physics [17]. The pseudoharmonic potential may be used for the energy spectrum of linear and non-linear systems [18]. The pseudoharmonic [8,9] and Mie-type [13-15] potentials are two exactly solvable potentials other than the Coulombic and anharmonic oscillator [9]. This paper is organized as follows. In Section 2, we solve analytically the  $D$ -dimensional radial Schrödinger equation with the molecular pseudoharmonic and modified Kratzer-Fues potentials. We also obtain the bound state eigensolutions of these molecular diatomic potentials by making a suitable ansatz to every wave function. The results are used to find energy spectra of diatomic  $N_2$ ,  $CO$ ,  $NO$  and  $CH$  molecules [15,19-20]. The concluding remarks will be given in Section 3.

## 2 The $D$ -Dimensional Radial Schrödinger Equation with Some Molecular Potentials

In the  $D$ -dimensional Hilbert space, the radial wave function  $\psi(r)$  of the Schrödinger equation can be written as [21]

$$\left[ \frac{d^2}{dr^2} + \frac{(D-1)}{r} \frac{d}{dr} - \frac{\ell(\ell+D-2)}{r^2} + \frac{2\mu}{\hbar^2} (E - V(r)) \right] \psi(r) = 0, \quad (1)$$

where  $\ell$  denotes the angular momentum quantum number and  $\mu$  is the reduced mass. Furthermore, to remove the first derivative from the above equation, we define a new radial wave function  $R(r)$  by means of equation

$$\psi(r) = r^{-(D-1)/2} R(r), \quad (2)$$

which will give the radial wave function  $R(r)$  satisfying the wave equation

$$\left\{ \frac{d^2}{dr^2} - \frac{[4\ell(\ell+D-2) + (D-1)(D-3)]}{4r^2} + \frac{2\mu}{\hbar^2} (E - V(r)) \right\} R(r) = 0. \quad (3)$$

Further, Equation (3) can be written into a simple analogy of the two-dimensional radial Schrödinger equation as [2,6]

$$\left\{ \frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2} (E - V(r)) - \frac{(\eta^2 - 1/4)}{r^2} \right\} R(r) = 0, \quad (4)$$

with the parameter

$$\eta = \ell + \frac{1}{2} (D - 2), \quad (5)$$

which is a linear combination of the spatial dimensions  $D$  and the angular momentum quantum number  $\ell$ .

### 2.1 The pseudoharmonic potential

This potential has been studied in three dimensions [8] using the polynomial solution method. It has the following form [8]

$$V(r) = D_e \left( \frac{r}{r_e} - \frac{r_e}{r} \right)^2, \quad (6)$$

which can be simply rewritten in the form of isotropic harmonic oscillator plus inverse quadratic potential [9] as

$$V(r) = ar^2 + \frac{b}{r^2} + c, \quad (7)$$

where  $a = D_e r_e^{-2}$ ,  $b = D_e r_e^2$  and  $c = -2D_e$ . We want to solve the radial SE, Eq. (4), with the potential given in Eq. (7) by taking an ansatz for the radial portion of wave function

$$R(r) = \exp[p(\alpha, r)] \sum_{n=0} a_n r^{2n+\delta+3/2}, \quad (8)$$

where

$$p(\alpha, r) = \frac{1}{2}\alpha r^2. \quad (9)$$

Substituting Eq. (8) into Eq. (4) and equating the coefficient of  $r^{2n+\delta+3/2}$  to zero, one can obtain

$$A_n a_n + B_{n+1} a_{n+1} + C_{n+2} a_{n+2} = 0, \quad (10)$$

where

$$A_n = \frac{2\mu}{\hbar^2} (E - c) + 2\alpha (2n + \delta + 2), \quad (11)$$

$$B_n = -\frac{2\mu b}{\hbar^2} - \left(\eta^2 - \frac{1}{4}\right) + \left(2n + \delta + \frac{3}{2}\right) \left(2n + \delta + \frac{1}{2}\right), \quad (12)$$

$$C_n = 0, \quad (13)$$

and the value of the parameter for  $p(\alpha, r)$  can be evaluated as

$$\alpha = \pm \sqrt{\frac{2\mu a}{\hbar^2}}. \quad (14)$$

To obtain a well-behaved solution at the origin and infinity, we must set  $\alpha = -\sqrt{\frac{2\mu a}{\hbar^2}}$  which ensures that wave function ansatz, Eq. (8), be finite for all  $r$ . Further, for a given  $p$ , if  $a_p \neq 0$ , but  $a_{p+1} = a_{p+2} = a_{p+3} = \dots = 0$ , we then obtain  $A_p = 0$  from Eq. (11), i.e.,

$$E_p^\delta = c + \sqrt{\frac{2\hbar^2 a}{\mu}} (2p + \delta + 2). \quad (15)$$

Carrying through a parallel analysis to Ref. [6],  $A_n$ ,  $B_n$  and  $C_n$  must satisfy the determinant relation for a nontrivial solution

$$\det \begin{vmatrix} B_0 & C_1 & \cdots & \cdots & \cdots & 0 \\ A_0 & B_1 & C_2 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & A_{p-1} & B_p \end{vmatrix} = 0. \quad (16)$$

To utilize this method, we present the exact solution for  $p = 0, 1$  as follows. (1): When  $p = 0$ , we can obtain from Eq. (15), the exact energy spectrum as

$$E_0^\delta = c + \sqrt{\frac{2\hbar^2 a}{\mu}} (\delta + 2). \quad (17)$$

Further, it is shown from Eq. (16) that  $B_0 = 0$ , which leads to the following restriction on the parameter  $\delta$  of the ansatz of wave function in Eq. (8) with  $\eta$  and potential parameters as

$$\delta = -1 + \sqrt{\frac{2\mu b}{\hbar^2} + \eta^2}. \quad (18)$$

It follows that the wave function for  $p = 0$  can be written as

$$\psi^{(0)}(r) = a_0 r^{\delta+2-D/2} \exp \left[ -\frac{1}{2} \sqrt{\frac{2\mu a}{\hbar^2}} r^2 \right], \quad (19)$$

where the normalization constant

$$a_0 = \sqrt{\frac{2}{(\delta+1)!}} \left( \sqrt{\frac{2\mu a}{\hbar^2}} \right)^{\delta/2+1}, \quad (20)$$

is determined from the requirement that

$$\int_0^\infty |\psi^{(n)}(r)|^2 r^{D-1} dr = 1. \quad (21)$$

(2): When  $p = 1$ , the exact energy spectrum becomes

$$E_1^\delta = c + \sqrt{\frac{2\hbar^2 a}{\mu}} (\delta + 4). \quad (22)$$

Furthermore, it is shown from Eq. (16) that  $B_0 B_1 = A_0 C_1$ , which leads to the restriction on  $\delta$  with the parameters of the potential and  $\eta$  as

$$\left( (\delta + 1)^2 - \eta^2 - \frac{2\mu b}{\hbar^2} \right) \left( (\delta + 3)^2 - \eta^2 - \frac{2\mu b}{\hbar^2} \right) = 0. \quad (23)$$

The wave function for  $p = 1$  can be read as

$$\psi^{(1)}(r) = (a_0 + a_1 r^2) r^{\delta+2-D/2} \exp \left[ -\frac{1}{2} \sqrt{\frac{2\mu a}{\hbar^2}} r^2 \right], \quad (24)$$

where  $a_0$  and  $a_1$  are normalization constants. The relation between them can be determined by Eqs (10)-(14) as

$$4\sqrt{\frac{2\mu a}{\hbar^2}} a_0 + \left( (\delta + 3)^2 - \eta^2 - \frac{2\mu b}{\hbar^2} \right) a_1 = 0, \quad (25)$$

which provides

$$a_1 = -\frac{1}{(\delta + 2)} \sqrt{\frac{2}{(\delta + 1)!}} \left( \sqrt{\frac{2\mu a}{\hbar^2}} \right)^{\delta/2+2}. \quad (26)$$

Following this way, we can generate a class of exact solutions through setting  $p = 0, 1, 2, \dots$ , etc. Generally speaking, if  $a_p \neq 0$ ,  $a_{p+1} = a_{p+2} = \dots = 0$ , we have  $A_p = 0$ , from which we can obtain the energy spectra (cf. Eq. (15)). The wave function can be read

$$\psi^{(p)}(r) = (a_0 + a_1 r^2 + \dots + a_p r^{2p}) r^{\delta+2-D/2} \exp \left[ -\frac{1}{2} \sqrt{\frac{2\mu a}{\hbar^2}} r^2 \right], \quad (27)$$

where  $a_i$  ( $i = 0, 1, 2, \dots, p$ ) are normalization constants.

(i) For the pseudoharmonic potential [8], with the parameters following Eq.(7), the exact energy spectra become

$$E_{n\ell} = -2D_e + \sqrt{\frac{\hbar^2 D_e}{2\mu r_e^2}} \left[ 4n + 2 + \sqrt{\frac{8\mu D_e r_e^2}{\hbar^2} + [2\ell + (D - 2)]^2} \right], \quad n, \ell = 0, 1, 2, \dots \quad (28)$$

and radial wave function becomes

$$\psi^{(n)}(r) = \left(a_0 + a_1 r^2 + \cdots + a_n r^{2n}\right) r^{-\frac{(D-2)}{2} + \sqrt{\frac{2\mu D_e r_e^2}{\hbar^2} + \left(\ell + \frac{(D-2)}{2}\right)^2}} \times \exp \left[ -\frac{1}{2} \sqrt{\frac{2\mu D_e}{\hbar^2 r_e^2}} r^2 \right]. \quad (29)$$

(ii) For the three dimensional ( $D = 3$ ) isotropic harmonic oscillator plus inverse quadratic potential [9],  $a = \frac{1}{2}\mu\omega^2$ ,  $b = g$  and  $c = 0$ , the exact energy spectra are

$$E_{n\ell} = \frac{\hbar\omega}{2} \left[ 4n + 2 + \sqrt{(2\ell + 1)^2 + \frac{8\mu g}{\hbar^2}} \right], n, \ell = 0, 1, 2, \dots, g > 0 \quad (30)$$

and the corresponding radial wave function in this case reads

$$\psi^{(n)}(r) = \left(a_0 + a_1 r^2 + \cdots + a_n r^{2n}\right) r^{-1 + \frac{1}{2} \left[ 1 + \sqrt{(2\ell + 1)^2 + \frac{8\mu g}{\hbar^2}} \right]} \exp \left[ -\frac{\mu\omega}{2\hbar} r^2 \right]. \quad (31)$$

where  $a_i$  with  $i = 0, 1, 2, \dots, n$  are normalization constants and  $\omega$  denotes the oscillator frequency. Its worthwhile to note that these results correspond to the results obtained by Ref. [9].

(iii) Also for  $a = B^2$  and  $b = c = 0$ , the potential in Eq. (7) turns to the anharmonic oscillator potential. And then its exact energy spectra are given as [8]

$$E_{n\ell} = \sqrt{\frac{\hbar^2}{2\mu}} B (4n + 2\ell + D), n, \ell = 0, 1, 2, \dots \quad (32)$$

and radial wave function becomes

$$\psi^{(n)}(r) = \left(a_0 + a_1 r^2 + \cdots + a_n r^{2n}\right) r^\ell \exp \left[ -\frac{1}{2} \sqrt{\frac{2\mu}{\hbar^2}} B r^2 \right], \quad (33)$$

where  $a_i$  with  $i = 0, 1, 2, \dots, n$  are normalization constants. On the other hand, setting  $\hbar = \mu = 1$ ,  $a = \frac{1}{2}$  and  $b = c = 0$ , gives the results of Ref. [22] for the results of exact harmonic oscillator energy states (cf. Eq. (8)) and wave functions (cf. after Eq.(4)).

## 2.2 The Mie-type potentials

This potential has been studied in the  $D$  dimensions using the polynomial solution method [14]. An example on this type of potentials is the standard Morse [10] or Kratzer-Fues [11,12] potential of the form [10-12]

$$V(r) = -D_e \left( \frac{2r_e}{r} - \frac{r_e^2}{r^2} \right), \quad (34)$$

where  $D_e$  is the dissociation energy between two atoms in a solid and  $r_e$  is the equilibrium internuclear separation. The standard Kratzer potential is modified by adding a  $D_e$  term to the potential. A new type of this potential is the modified Kratzer-type of molecular potential [15]

$$V(r) = D_e \left( \frac{r - r_e}{r} \right)^2, \quad (35)$$

and hence it is shifted in amount of  $D_e$ . The potential in Eq. (35) will be studied in  $D$  dimensions by making the wave function ansatz [6]. However, this potential has also been discussed before in three dimensions [15] and in  $D$  dimensions [14]. This potential [13] can be simply taken as

$$V(r) = \frac{a}{r} + \frac{b}{r^2} + c, \quad (36)$$

where  $a = -D_e r_e$ ,  $b = D_e r_e^2$  and  $c = D_e$  [15].

We take the following ansatz for the radial wave function

$$R(r) = \exp[p(\alpha, r)] \sum_{n=0} a_n r^{n+\delta+1/2}, \quad (37)$$

where

$$p(\alpha, r) = \alpha r. \quad (38)$$

Substituting Eq. (36) into Eq. (4) and setting the coefficient of  $r^{n+\delta-1/2}$  to zero, we have

$$A_n a_n + B_{n+1} a_{n+1} + C_{n+2} a_{n+2} = 0, \quad (39)$$

where

$$A_n = -\frac{2\mu a}{\hbar^2} + 2\alpha \left( n + \delta + \frac{1}{2} \right), \quad (40)$$



$$B_n = -\frac{2\mu b}{\hbar^2} - \left(\eta^2 - \frac{1}{4}\right) + \left(n + \delta + \frac{1}{2}\right) \left(n + \delta - \frac{1}{2}\right), \quad (41)$$

$$C_n = 0, \quad (42)$$

and the value of the parameter for  $p$  ( $\alpha, r$ ) can be evaluated as

$$\alpha^2 = -\frac{2\mu}{\hbar^2}(E - c), \quad (43)$$

from which we must set

$$\alpha = -\sqrt{-\frac{2\mu}{\hbar^2}(E - c)}, E < c. \quad (44)$$

which ensures that wave function ansatz Eq. (37) be finite for all  $r$ . This is required by the physically acceptable solution. On the other hand, for a given  $p$ , if  $a_p \neq 0$ , but  $a_{p+1} = a_{p+2} = a_{p+3} = \dots = 0$ , it is easy to obtain  $A_p = 0$  from Eq. (40), i.e.,

$$E_p^\delta = c - \frac{\mu a^2}{2\hbar^2 \left(p + \delta + \frac{1}{2}\right)^2}. \quad (45)$$

To apply this method, we will give the exact solutions for  $p = 0, 1$  below.

(1): When  $p = 0$ , it is found from Eq. (45) that the exact energy spectrum becomes

$$E_0^\delta = c - \frac{\mu a^2}{2\hbar^2 \left(\delta + \frac{1}{2}\right)^2}. \quad (46)$$

The restriction on the parameter  $\delta$  with potential parameters and  $\eta$  can be obtained from  $B_0 = 0$  as

$$\delta = \sqrt{\frac{2\mu b}{\hbar^2} + \eta^2}. \quad (47)$$

The wave function for  $p = 0$  now becomes

$$\psi^{(0)}(r) = a_0 r^{\delta - \frac{(D-2)}{2}} \exp \left[ -\sqrt{-\frac{2\mu}{\hbar^2}(E - c)} r \right], E < c, \quad (48)$$

where

$$a_0 = \frac{1}{\sqrt{(2\delta+1)!}} \left( 2\sqrt{-\frac{2\mu}{\hbar^2}(E-c)} \right)^{\delta+1}, \quad (49)$$

is a normalization constant obtained via Eq. (21).

(2): When  $p = 1$ , the exact energy spectrum becomes

$$E_1^\delta = c - \frac{\mu a^2}{2\hbar^2 \left(\delta + \frac{3}{2}\right)^2}. \quad (50)$$

It is shown that the restriction on the parameter  $\delta$  with of the potential parameters and  $\eta$  can be obtained from  $B_0 B_1 = A_0 C_1$

$$\left( (\delta+1)^2 - \eta^2 - \frac{2\mu b}{\hbar^2} \right) \left( \delta^2 - \eta^2 - \frac{2\mu b}{\hbar^2} \right) = 0. \quad (51)$$

The wave function for  $p = 1$  becomes

$$\psi^{(1)}(r) = (a_0 + a_1 r) r^{\delta-(D-2)/2} \exp \left[ -\sqrt{-\frac{2\mu}{\hbar^2}(E-c)} r \right], E < c, \quad (52)$$

where the relation between them can be found as

$$-\frac{4\mu a}{\hbar^2} \left( \frac{\delta+1}{\delta+\frac{3}{2}} \right) a_0 + (2\delta+1) a_1 = 0, \quad (53)$$

which provides

$$a_1 = \frac{8\mu a}{\hbar^2} \frac{(\delta+1)}{(2\delta+3)(2\delta+1)\sqrt{(2\delta+1)!}} \left( 2\sqrt{-\frac{2\mu}{\hbar^2}(E-c)} \right)^{\delta+1}, E < c. \quad (54)$$

Following this way, we can generate a class of exact solutions through setting  $p = 0, 1, 2, \dots$ , etc. Generally speaking, if  $a_p \neq 0$ ,  $a_{p+1} = a_{p+2} = \dots = 0$ , we have  $A_p = 0$ , from which we can obtain the energy spectra (cf. Eq. (45)). The corresponding wave function can also be read as

$$\psi^{(p)}(r) = (a_0 + a_1 r + \dots + a_p r^p) r^{-\frac{(D-2)}{2} + \sqrt{\frac{2\mu b}{\hbar^2} + \left(\ell + \frac{(D-2)}{2}\right)^2}}$$

$$\times \exp \left[ -\sqrt{-\frac{2\mu}{\hbar^2}(E - c)}r \right], E < c \quad (55)$$

where  $a_i$  ( $i = 0, 1, 2, \dots, p$ ) are normalization constants.

(i) For the standard Kratzer-Fues (Mie-type) potential [14], with the parameters  $a = -D_e r_e$ ,  $b = D_e r_e^2$  and  $c = 0$ , the exact energy spectra are given as (cf. Ref. [14])

$$E_{n\ell} = -\frac{\hbar^2}{2\mu} \left[ \left( \frac{4\mu D_e r_e}{\hbar^2} \right)^2 \left( 2n + 1 + \sqrt{\frac{8\mu D_e r_e^2}{\hbar^2} + [2\ell + D - 2]^2} \right)^{-2} \right], \quad (56)$$

and the corresponding radial wave function becomes

$$\begin{aligned} \psi^{(n)}(r) &= (a_0 + a_1 r + \dots + a_n r^n) r^{-\frac{(D-2)}{2} + \frac{1}{2} \sqrt{\frac{8\mu D_e r_e^2}{\hbar^2} + (2\ell + D - 2)^2}} \\ &\times \exp \left[ -\sqrt{-\frac{2\mu}{\hbar^2} E_{n\ell}} r \right], E_{n\ell} < 0. \end{aligned} \quad (57)$$

(ii) For the modified Kratzer potential [15], with the parameters following Eq. (36), the exact energy spectra are given as (cf. Ref. [15])

$$E_{n\ell} = D_e - \frac{\hbar^2}{2\mu} \left[ \left( \frac{4\mu D_e r_e}{\hbar^2} \right)^2 \left( 2n + 1 + \sqrt{\frac{8\mu D_e r_e^2}{\hbar^2} + [2\ell + D - 2]^2} \right)^{-2} \right], \quad (58)$$

and the radial wave function becomes

$$\begin{aligned} \psi^{(n)}(r) &= (a_0 + a_1 r + \dots + a_n r^n) r^{-\frac{(D-2)}{2} + \frac{1}{2} \sqrt{\frac{8\mu D_e r_e^2}{\hbar^2} + (2\ell + D - 2)^2}} \\ &\times \exp \left[ -\sqrt{-\frac{2\mu}{\hbar^2} (E_{n\ell} - D_e)} r \right], E_{n\ell} < D_e. \end{aligned} \quad (59)$$

(iii) Also after setting  $a = -A$  and  $b = c = 0$ , the potential in Eq. (36) turns to the Coulomb potential. Then its exact energy spectra are given as [23]

$$E_{n\ell} = -\frac{\mu A^2}{2\hbar^2 \left( n + \ell + \frac{(D-1)}{2} \right)^2}, \quad (60)$$

and thus the radial wave function reads

$$\psi^{(n)}(r) = \left(a_0 + a_1 r^2 + \cdots + a_n r^n\right) r^\ell \exp \left[ -\sqrt{-\frac{2\mu}{\hbar^2} E_n} r \right], \quad (61)$$

where  $a_i$  with  $i = 0, 1, 2, \dots, n$  are normalization constants.

### 3 Concluding Remarks

We have easily obtained the exact bound state solutions of the  $D$  dimensional radial Schrödinger equation for a diatomic molecule with two general potential forms representing the pseudoharmonic [8] and modified Kratzer molecular [15] potentials by using the wave function ansatz method [6]. The presented procedure in this study is systematical and efficient in finding the exact energy spectra and corresponding wave functions of the Schrödinger equation for various diatomic molecules. This new method is tested to calculate the energy spectra of the  $N_2$ ,  $CO$ ,  $NO$  and  $CH$  molecules and our numerical calculations are similar to those given in Table II with parameter values shown in Table I (cf. Ref. [8]) for pseudoharmonic potential and also to the ones given by Ref. [15] with the modified Kratzer potential for the given quantum numbers  $n = 0, 1, 2, 3, 4, 5$ . This method is simple and promising in producing the exact bound state solution for further anharmonic potentials [6], quarkonium potentials [21] and inter-nuclear potentials [24].

### 4 Acknowledgments

This research was partially supported by the Scientific and Technological Research Council of Turkey. S.M. Ikhdair is grateful to Dr. Suat Günsel, founder president of NEU, for a partial fund.

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